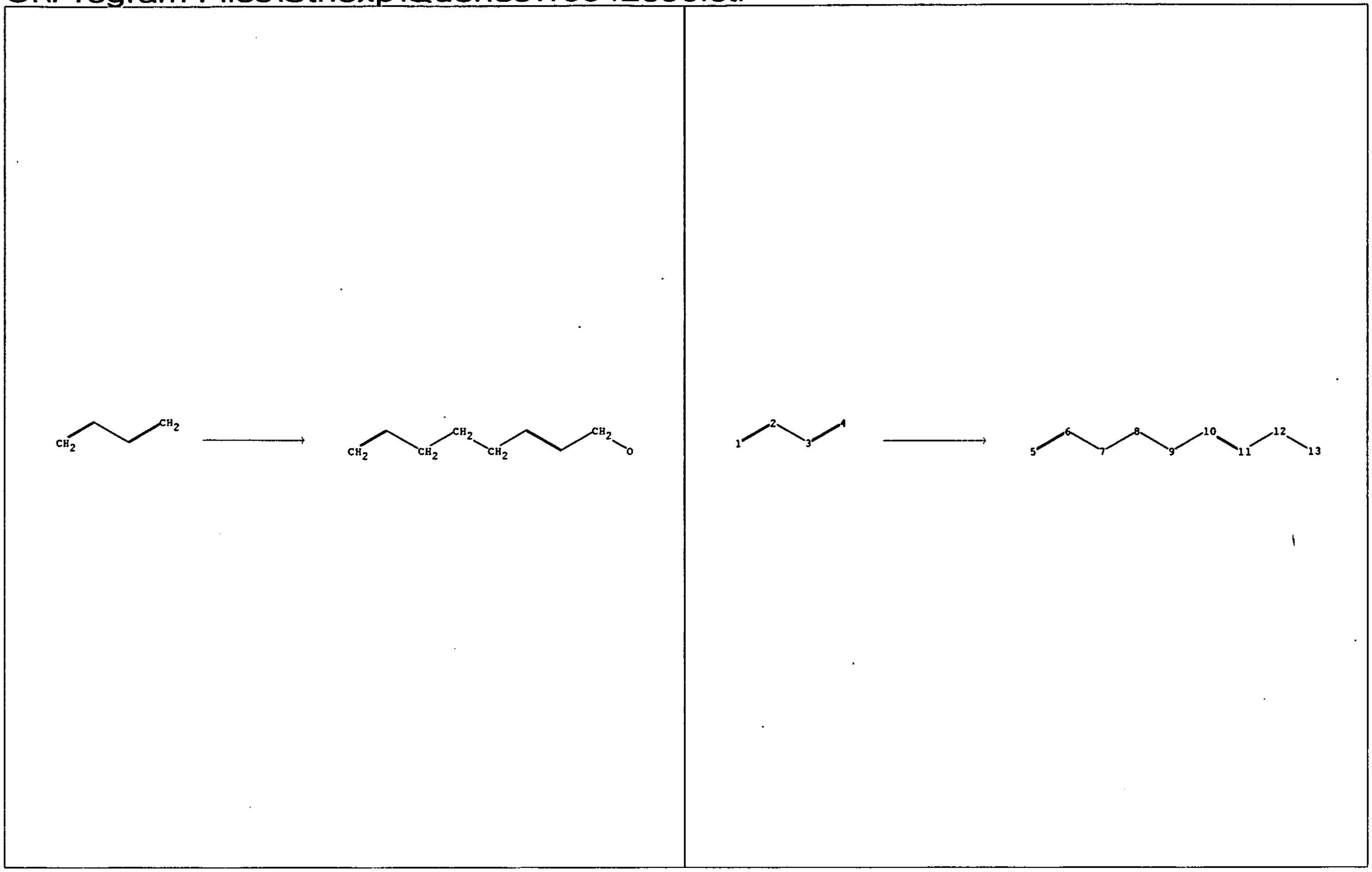
C:\Program Files\Stnexp\Queries\10542890.str



chain nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds :
    1-2 2-3 3-4 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13
exact bonds :
    1-2 2-3 3-4 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13

Match level :
    1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS9:CLASS
    10:CLASS11:CLASS12:CLASS13:CLASS
fragments assigned product role:
    containing 5
fragments assigned reactant/reagent role:
    containing 1

```
* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:54:39 ON 23 FEB 2007

=> file casreact
COST IN U.S. DOLLARS                              SINCE FILE     TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST                                     0.21      0.21

FILE 'CASREACT' ENTERED AT 09:55:02 ON 23 FEB 2007
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FILE CONTENT:1840 - 18 Feb 2007 VOL 146 ISS 8

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************************************************************
*                                                          *
*     CASREACT now has more than 12 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10542890.str

L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 09:55:21 FILE 'CASREACT'
SCREENING COMPLETE -     2497 REACTIONS TO VERIFY FROM      184 DOCUMENTS

100.0% DONE    2497 VERIFIED       3 HIT RXNS                     3 DOCS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:      46948 TO    52932
PROJECTED ANSWERS:                3 TO      163

L2            3 SEA SSS SAM L1 (      3 REACTIONS)
```

=> d l2 1-3

L2 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2$ $\xrightarrow[\text{C:14024-64-7, t-BuOH, Water}]{\text{Pd(OAc)2, C:110107-24-9,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$
25%

REF: Jpn. Kokai Tokkyo Koho, 09059193, 04 Mar 1997, Heisei

L2 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2$ $\xrightarrow[\text{CO2, Water, Me2CO}]{\text{Pd(OAc)2, Tri-o-tolylphosphine,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$

REF: Jpn. Kokai Tokkyo Koho, 06287156, 11 Oct 1994, Heisei

L2 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 2

$H_3C{-}OH$ $\xrightarrow[\text{C:148800-96-8, PPh3}]{\text{1,3-Butadiene,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OMe$ +

$H_2C{=}CH{-}CH(OMe){-}(CH_2)_3{-}CH{=}CH_2$ +

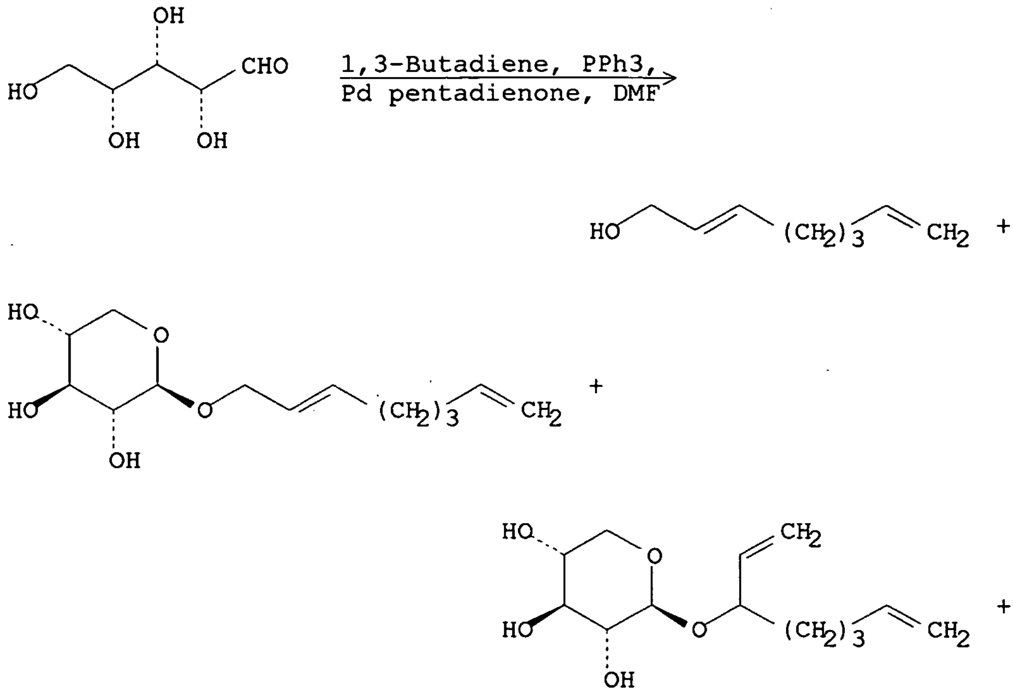
STRUCTURE
DIAGRAM
IS NOT
AVAILABLE
26952-74-9

REF: Jpn. Kokai Tokkyo Koho, 04327594, 17 Nov 1992, Heisei
NOTE: 60.degree. under N2

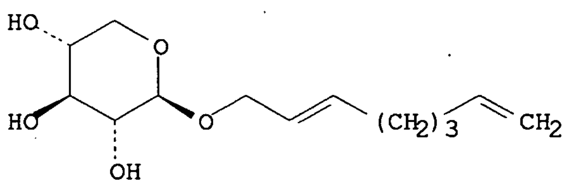
```
=> s l1 ful
FULL SEARCH INITIATED 09:56:07 FILE 'CASREACT'
SCREENING COMPLETE -      54480 REACTIONS TO VERIFY FROM       3626 DOCUMENTS

100.0% DONE    54480 VERIFIED      180 HIT RXNS                        68 DOCS
SEARCH TIME: 00.00.07

L3            68 SEA SSS FUL L1 (    180 REACTIONS)

=> d l3 1-68
```

L3 ANSWER 1 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 11



RX(1) OF 11



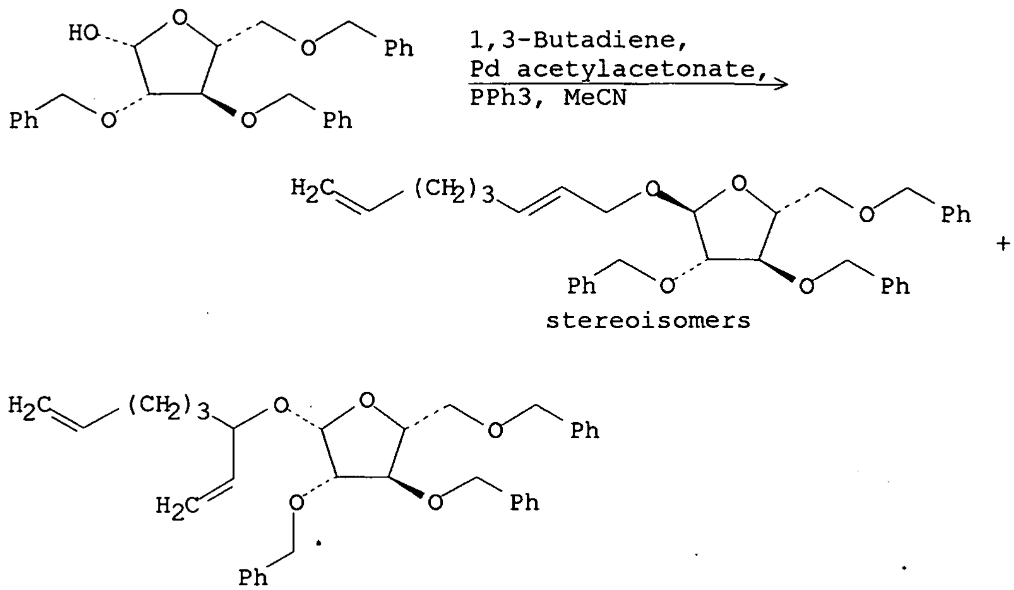
REF: Journal of Molecular Catalysis A: Chemical, 238(1-2), 199-206; 2005

NOTE: chemoselective, regioselective, stereoselective, 30:70 alpha:beta, 8:1 E:Z, optimization study, optimized on amount of butadiene, optimized on reaction time, product depends on reaction conditions

CON: 70 hours, 20 deg C

L3 ANSWER 2 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 4



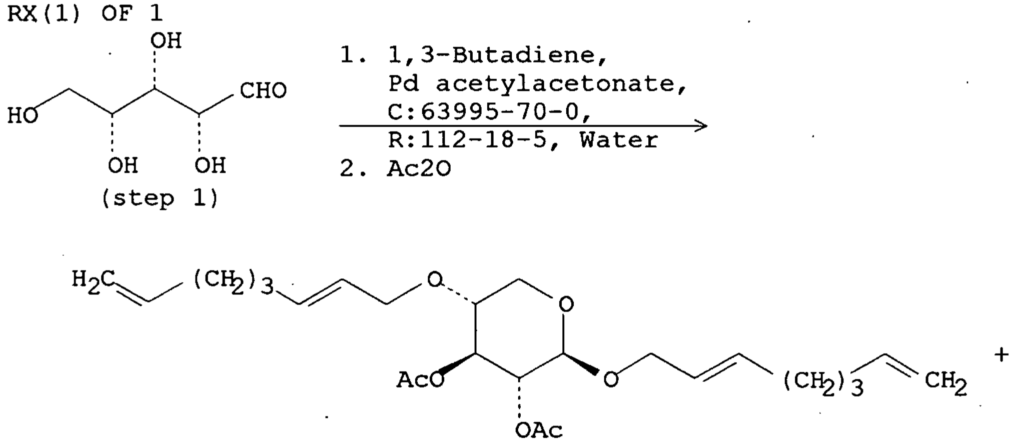
REF: Carbohydrate Research, 2006, 341(1), 153-159; 2005

NOTE: 99% overall yield, alternative reaction conditions gave lower yield, autoclave used, optimization study

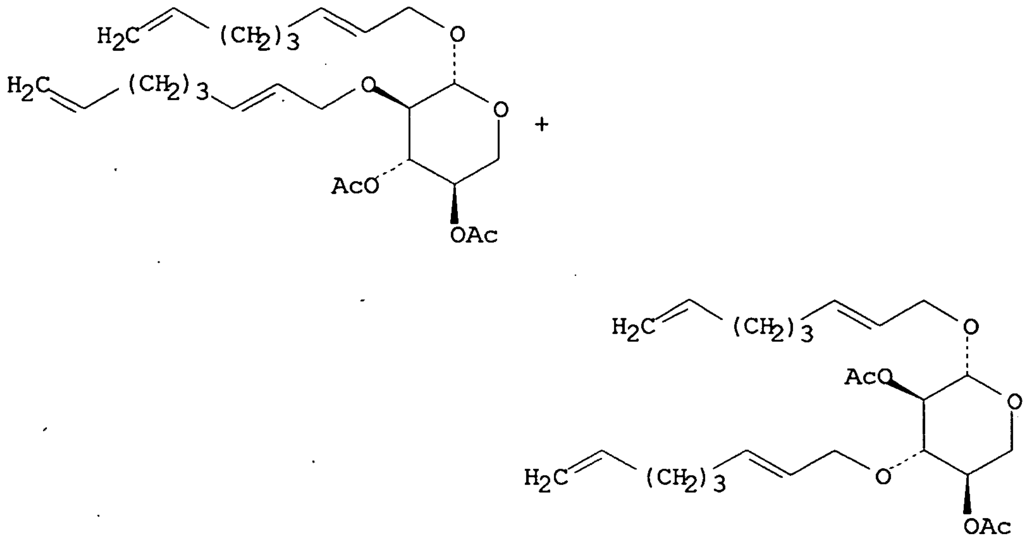
CON: 24 hours, 75 deg C

L3 ANSWER 3 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1



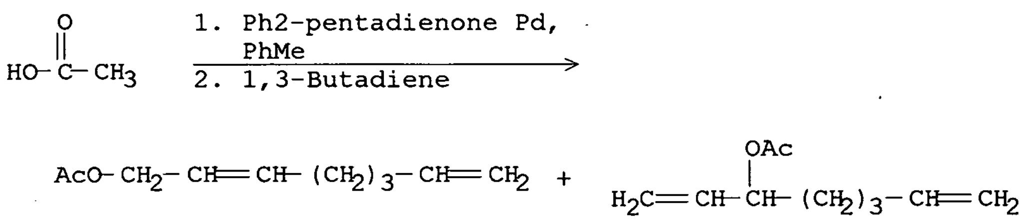
RX(1) OF 1



REF: Green Chemistry, 7(4), 219-223; 2005
NOTE: stereoselective, 83% conversion, Et3N and DIPEA gave lower conversion, optimization study, optimized on base, reactant assumed in 2nd stage
CON: 45 minutes, 80 deg C

L3 ANSWER 4 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

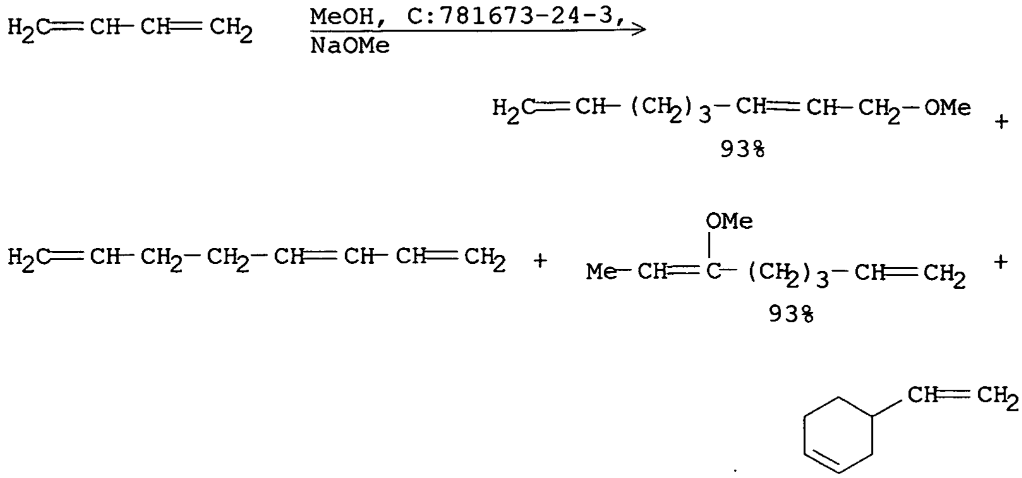
RX(1) OF 1



REF: U.S. Pat. Appl. Publ., 2005038305, 17 Feb 2005
NOTE: optimization study, regioselective
CON: STAGE(1) 0.17 hours, 25 deg C; 25 deg C -> -60 deg C
STAGE(2) 215 deg C; 8 hours, 25 deg C -> 60 deg C

L3 ANSWER 5 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

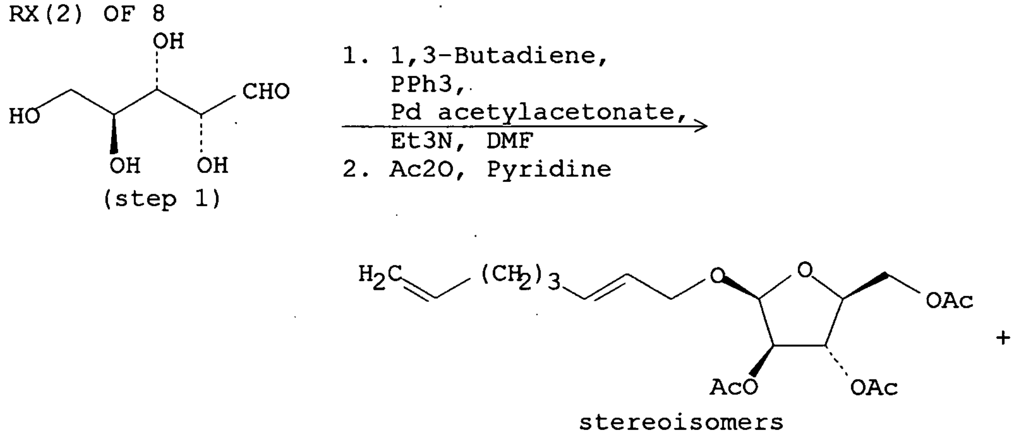
RX(6) OF 28



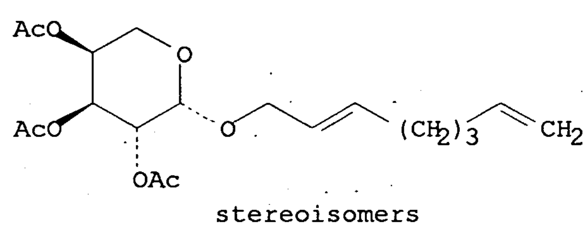
REF: Chemistry--A European Journal, 10(16), 3891-3900; 2004
NOTE: chemoselective, regioselective, alternative catalysts gave lower yields, stainless steel Parr autoclave used
CON: STAGE(1) -78 deg C; -78 deg C -> 70 deg C; 16 hours, 70 deg C

L3 ANSWER 6 OF 68 CASREACT

RX(2) OF 8



RX(2) OF 8



REF: European Journal of Organic Chemistry, (13), 2914-2922; 2004
NOTE: other products also detected, stereoselective, isomer mix; 86% overall yield ; selectivity depends on time,additive , cat. and amt. of amine and phosphine
CON: STAGE(1) 45 minutes, 75 deg C; cooled
STAGE(2) 12 hours, room temperature

L3 ANSWER 7 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3

$HO-CH_2-CH_2-CH_2-OH \xrightarrow[\text{Pd(OAc)2, Water}]{\text{1,3-Butadiene, C:63995-70-0,}}$

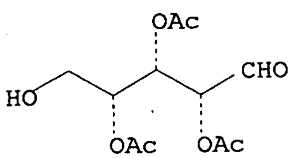
$H_2C{=}CH-(CH_2)_3-CH{=}CH-CH_2-O-(CH_2)_3-OH$

56%

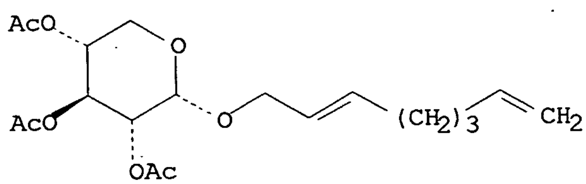
REF: Advanced Synthesis & Catalysis, 345(11), 1242-1246; 2003
NOTE: autoclave used, other product also detected, yield depends on reaction conditions
CON: 4 hours, 80 deg C, 10 bar -> 5 bar

L3 ANSWER 8 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 5



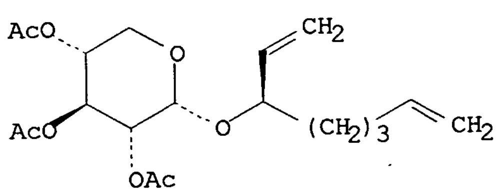
1,3-Butadiene,
Pd acetylacetonate, →
PPh3, THF



+

stereoisomers

RX(1) OF 5

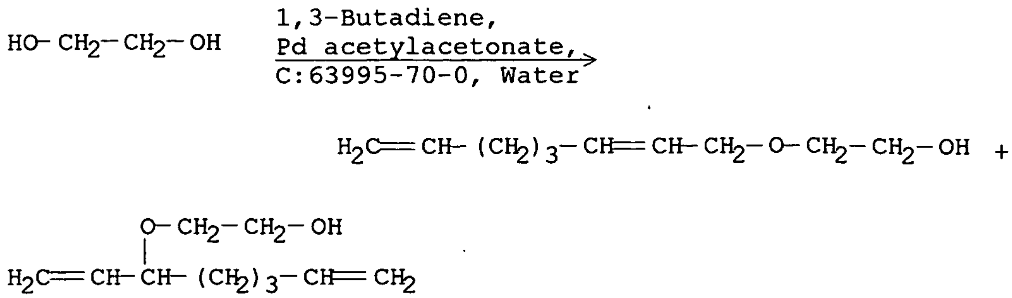


stereoisomers

REF: European Journal of Organic Chemistry, (3), 511-520; 2004
NOTE: regioselective, stereoselective, 49:51 alpha:beta, 97 % overall yield;autoclave used;optimization study;optimized on solvent used;other solvents(DMF,DCM and MeCN) gave lower yield and regioselectivity;yield proportions determined by GC;;%
CON: 4 hours, 70 deg C

L3 ANSWER 9 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

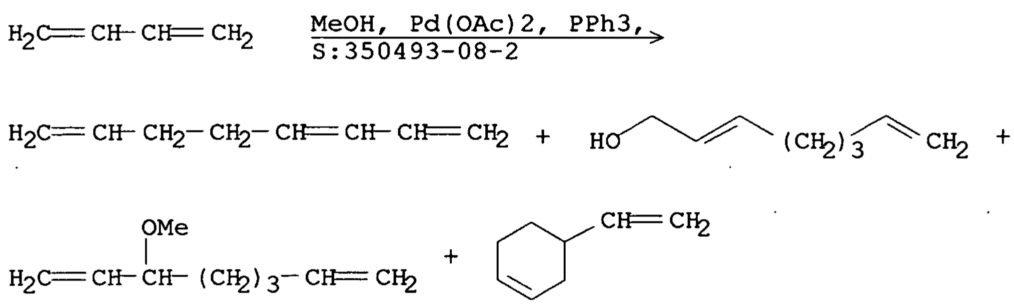
RX(3) OF 7



REF: Green Chemistry, 5(2), 198-204; 2003
NOTE: 75 % overall yield;green chem.-renewable feedstock;high pressure; other products also detected;selective to monotelomers;stainless steel autoclave used%
CON: STAGE(1) room temperature; room temperature -> 80 deg C; 4 hours, 80 deg C, 10 bar

L3 ANSWER 10 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

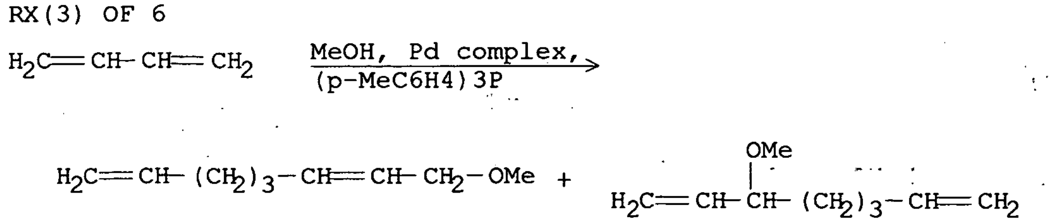
RX(1) OF 15



REF: Organometallics, 22(22), 4418-4425; 2003
NOTE: ionic liq., product distribution depends on solvent, ligand, other products also detected, 100% conversion
CON: STAGE(1) -10 deg C; 1 hour, 85 deg C

L3 ANSWER 11 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 6



REF: European Journal of Organic Chemistry, (2), 274-283; 2003
NOTE: regioselective, other products also detected (butadiene dimers), optimization study of catalyst
CON: STAGE(1) room temperature; room temperature -> -20 deg C; -20 deg C; .75 hours, 60 deg C, 4 bar

L3 ANSWER 12 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 4

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{NaOH}]{\text{MeOH, C:441018-46-8,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OMe$ + $H_2C{=}CH{-}CH(OMe){-}(CH_2)_3{-}CH{=}CH_2$

REF: Angewandte Chemie, International Edition, 41(6), 986-989; 2002
NOTE: 98% overall, chemoselective

L3 ANSWER 13 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(5) OF 15

$HO{-}(CH_2)_6{-}OH \xrightarrow[\text{Pd(OAc)2, PPh3, H2}]{\text{1,3-Butadiene,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}O{-}(CH_2)_6{-}OH$

REF: Jpn. Kokai Tokkyo Koho, 2002020343, 23 Jan 2002

L3 ANSWER 14 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 10

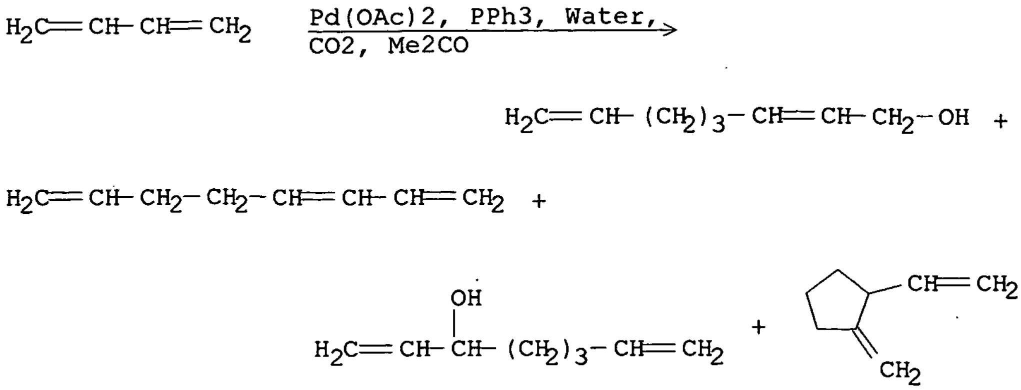
$MeO{-}C({=}O){-}(CH_2)_5{-}OH \xrightarrow[\text{Pd(OAc)2}]{\text{1,3-Butadiene, PBu3,}}$

$MeO{-}C({=}O){-}(CH_2)_5{-}O{-}CH_2{-}CH{=}CH{-}(CH_2)_3{-}CH{=}CH_2$
66%

REF: Jpn. Kokai Tokkyo Koho, 2001240598, 04 Sep 2001

L3 ANSWER 15 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

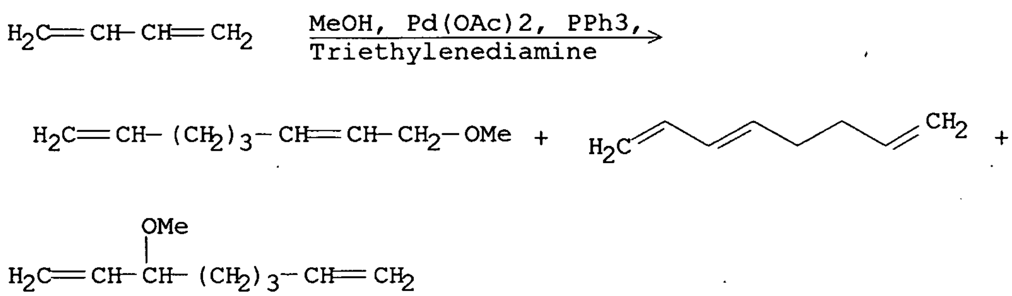
RX(1) OF 1



REF: Journal of Molecular Catalysis A: Chemical, 166(2), 233-242; 2001
NOTE: products and the ratio related cat

L3 ANSWER 16 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

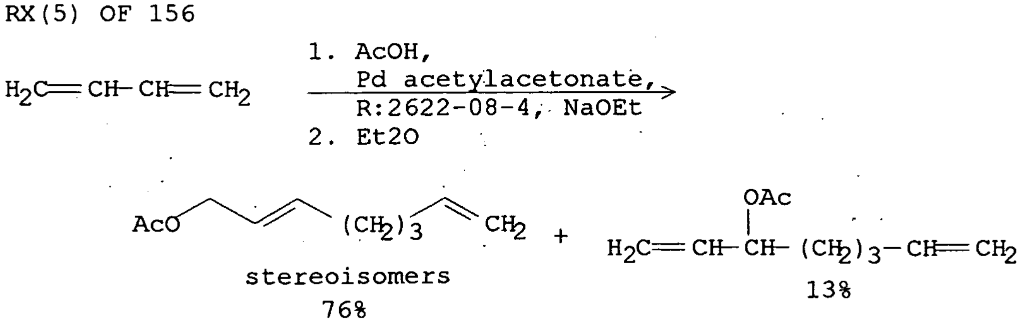
RX(1) OF 1



REF: Advanced Synthesis & Catalysis, 343(1), 29-33; 2001
NOTE: 80% conversion

L3 ANSWER 17 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(5) OF 156



REF: European Journal of Organic Chemistry, (17), 2991-3000; 2000

L3 ANSWER 18 OF 68 CASREACT

RX(1) OF 1

$$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{CO2, Water, Me2CO}]{\text{Pd(OAc)2, Tri-o-tolylphosphine,}}$$

$$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH \; + \; H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2$$

REF: Jpn. Kokai Tokkyo Koho, 11189556, 13 Jul 1999, Heisei
NOTE: 75.degree. for 3 h; 1,7-octadien-3-ol/2,7-octadiene-1-ol ratio of 20.3

L3 ANSWER 19 OF 68 CASREACT

RX(1) OF 1

$$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{Water, Me2CO}]{\text{Pd(OAc)2, C:213543-25-0, CO2,}}$$

$$\underset{70\%}{H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH} \; + \; \underset{3\%}{H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2}$$

REF: Jpn. Kokai Tokkyo Koho, 10237082, 08 Sep 1998, Heisei

L3 ANSWER 20 OF 68 CASREACT

RX(1) OF 5

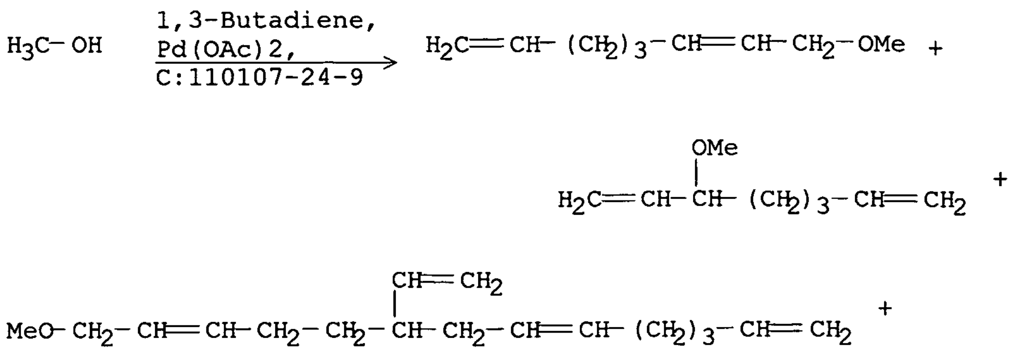
$$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{PEt3, Hexane}]{\text{MeOH, Pd pentadienone,}}$$

$$\underset{98\%}{H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OMe}$$

REF: Journal of Molecular Catalysis A: Chemical, 129(2-3), 179-189; 1998
NOTE: seeking to suppress trimer and dimer formation; excess alc. required, phosphine has little effect

L3 ANSWER 21 OF 68 CASREACT

RX(2) OF 2

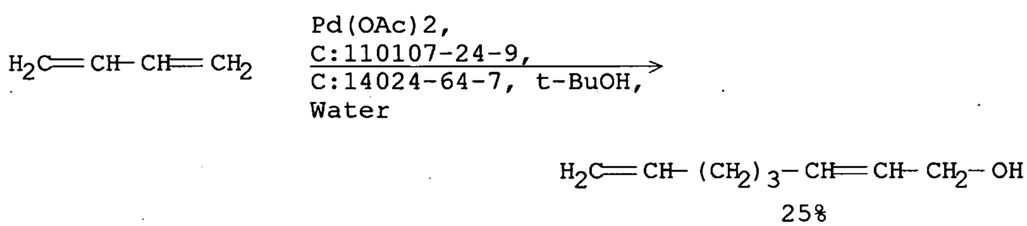


MULTI
PAGE
IMAGE
192522-71-7

REF: Jpn. Kokai Tokkyo Koho, 09176051, 08 Jul 1997, Heisei
NOTE: heating to 90.degree. over 20 min and at 90.degree. for 30 min

L3 ANSWER 22 OF 68 CASREACT

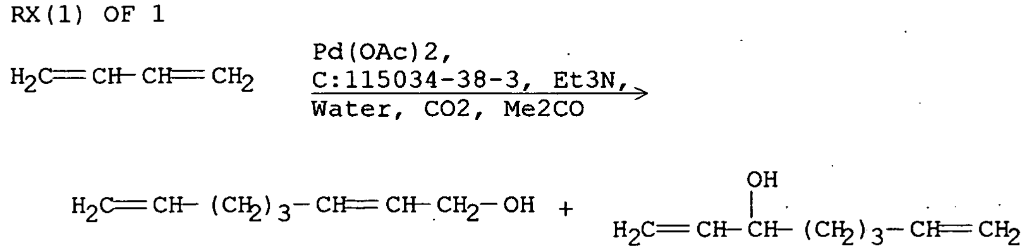
RX(1) OF 1



REF: Jpn. Kokai Tokkyo Koho, 09059193, 04 Mar 1997, Heisei

L3 ANSWER 23 OF 68 CASREACT

RX(1) OF 1



REF: Ger. Offen., 19547498, 27 Jun 1996

L3 ANSWER 24 OF 68 CASREACT

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{Water, Me2CO}]{\text{Pd(OAc)2, C:110107-24-9, CO2,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$ 52% + $H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2$ 4%

REF: Ger. Offen., 19523335, 04 Jan 1996

L3 ANSWER 25 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{C:112-18-5, CO2, Water}]{\text{Pd(OAc)2, C:160583-34-6,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$

REF: PCT Int. Appl., 9530636, 16 Nov 1995

L3 ANSWER 26 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{Pd(OAc)2, Water}]{\text{C:63995-75-5, C:157978-20-6, Et3N,}}$

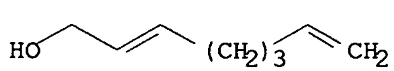
$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$ 54% + $H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2$ 54%

REF: PCT Int. Appl., 9526948, 12 Oct 1995

L3 ANSWER 27 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{MeCN; 2. CO2, Water}]{\text{1. Tri-o-tolylphosphine, Pd acetylacetonate,}}$



+ $H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2$

REF: Journal of the Chemical Society, Chemical Communications, (9), 931-2; 1995
NOTE: 27% OVERALL YIELD, NATURE OF CATALYST AND REACTION TEMP. DETERMINE PRODUCT DISTRIBUTION

L3 ANSWER 28 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{CO2, Water, Me2CO}]{\text{Pd(OAc)2, Tri-o-tolylphosphine,}} H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$

REF: Jpn. Kokai Tokkyo Koho, 06287156, 11 Oct 1994, Heisei

L3 ANSWER 29 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{CO2, Water, Me2CO}]{\text{Pd(OAc)2, Tri-o-tolylphosphine,}} H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$

REF: Jpn. Kokai Tokkyo Koho, 06287155, 11 Oct 1994, Heisei

L3 ANSWER 30 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{CO2, Water, Me2CO}]{\text{Pd(OAc)2, Tri-o-tolylphosphine,}} H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$

REF: Ger. Offen., 4410746, 06 Oct 1994

L3 ANSWER 31 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{PPh3, Water}]{\text{Pd acetylacetonate,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH \; + \; H_2C{=}CH{-}\underset{}{\overset{OH}{\overset{|}{CH}}}{-}(CH_2)_3{-}CH{=}CH_2$

REF: PCT Int. Appl., 9400410, 06 Jan 1994
NOTE: CO2 pressure 20 kg/cm2; 90.degree.

L3 ANSWER 32 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

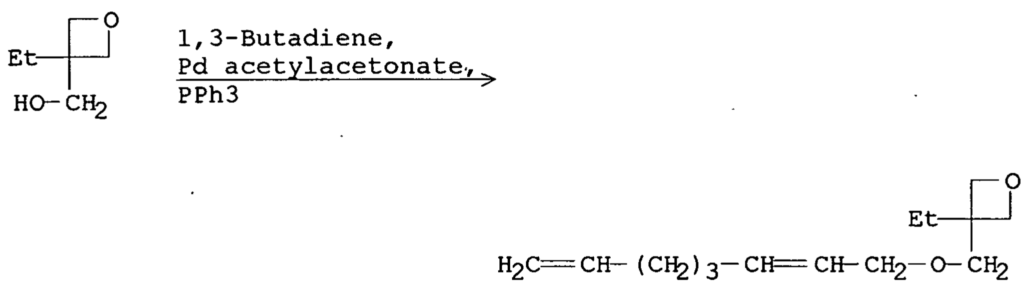
$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{Water, CO2, DMF}]{\text{PPh3, C:29335-52-2,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH \;+\; H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2$

REF: Jpn. Kokai Tokkyo Koho, 05155795, 22 Jun 1993, Heisei
NOTE: 90.degree., 3 h; 78% butadiene conversion; 74% selectivity for 2, 4-octadienol.

L3 ANSWER 33 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 2



REF: Eur. Pat. Appl., 546422, 16 Jun 1993
NOTE: no solvent

L3 ANSWER 34 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{CO2, Me2CO}]{\text{Pd(OAc)2, C:133833-71-3, Water,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$
84%

REF: Brit. UK Pat. Appl., 2260136, 07 Apr 1993

L3 ANSWER 35 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 2

$H_3C-OH \xrightarrow[\text{C:148800-96-8, PPh3}]{\text{1,3-Butadiene,}}$

$H_2C{=}CH-(CH_2)_3-CH{=}CH-CH_2-OMe$ +

$H_2C{=}CH-CH(OMe)-(CH_2)_3-CH{=}CH_2$ + STRUCTURE DIAGRAM IS NOT AVAILABLE 26952-74-9

REF: Jpn. Kokai Tokkyo Koho, 04327594, 17 Nov 1992, Heisei
NOTE: 60.degree. under N2

L3 ANSWER 36 OF 68 CASREACT

RX(1) OF 1

$H_3C-OH \xrightarrow[\text{C:304-88-1, Pd, PPh3}]{\text{1,3-Butadiene,}}$

$H_2C{=}CH-(CH_2)_3-CH{=}CH-CH_2-OMe$ + $H_2C{=}CH-CH(OMe)-(CH_2)_3-CH{=}CH_2$

REF: Jpn. Kokai Tokkyo Koho, 04327552, 17 Nov 1992, Heisei

L3 ANSWER 37 OF 68 CASREACT

RX(1) OF 1

$H_2C{=}CH-CH{=}CH_2 \xrightarrow[\text{CO2, MeCN}]{\text{Pd acetylacetonate, PPh3, C:9003-39-8,}}$

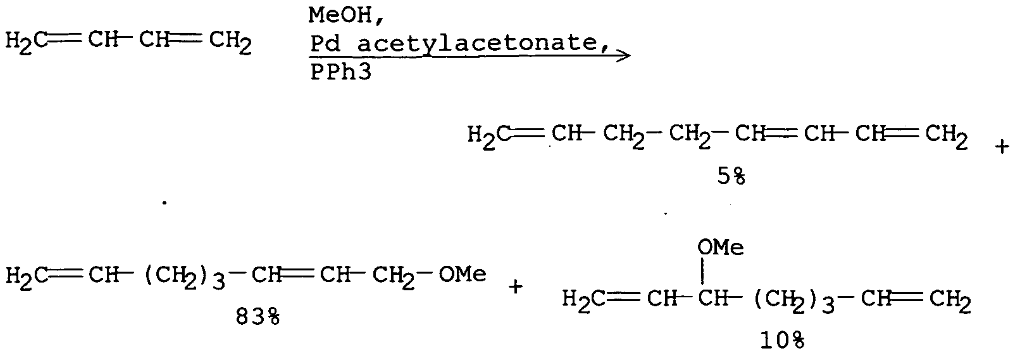
$H_2C{=}CH-(CH_2)_3-CH{=}CH-CH_2-OH$ (51%) + $Me-(CH_2)_6-Me$ (29%) +

$H_2C{=}CH-CH(OH)-(CH_2)_3-CH{=}CH_2$ (20%)

REF: U.S., 5169981, 08 Dec 1992

L3 ANSWER 38 OF 68 CASREACT

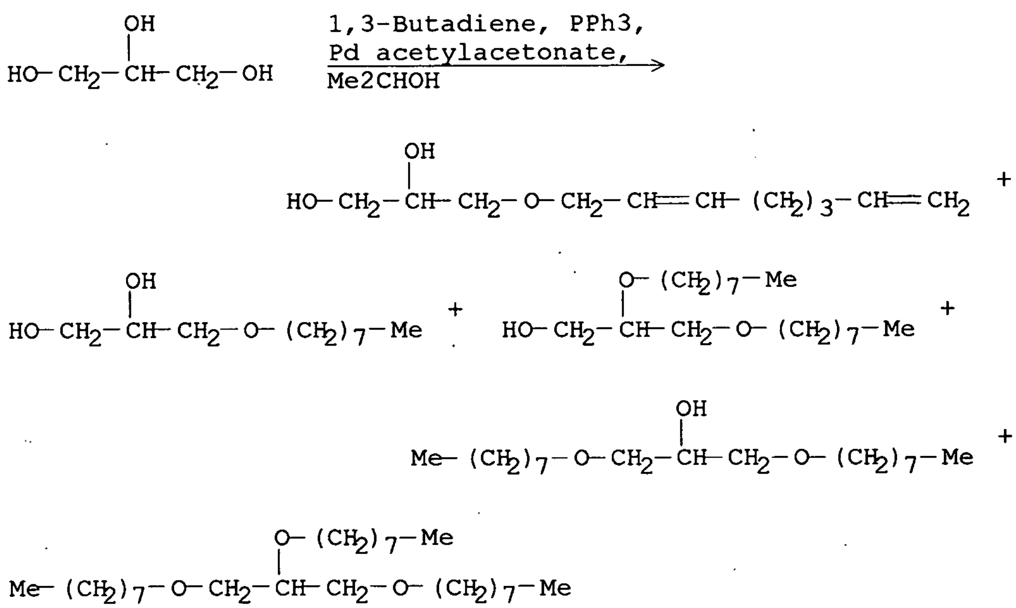
RX(1) OF 1



REF: Fenzi Cuihua, 6(2), 148-55; 1992

L3 ANSWER 39 OF 68 CASREACT

RX(1) OF 3



REF: Ger. Offen., 4021015, 09 Jan 1992

L3 ANSWER 40 OF 68 CASREACT

RX(1) OF 1

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{Water}]{\text{Pd acetylacetonate, PPh3, Ph3P(O), CO2,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OH$ + $H_2C{=}CH{-}CH(OH){-}(CH_2)_3{-}CH{=}CH_2$

REF: Ger. Offen., 3925217, 31 Jan 1991
NOTE: 93% overall

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RX(10) OF 12

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow[\text{NaOPh, MeOH, THF}]{\text{Pd acetylacetonate, C:26222-40-2, PPh3,}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OMe$ +

$H_2C{=}CH{-}CH_2{-}CH_2{-}CH{=}CH{-}CH{=}CH_2$ + $H_2C{=}CH{-}CH(OMe){-}(CH_2)_3{-}CH{=}CH_2$

REF: Journal of Molecular Catalysis, 55(1-3), 340-52; 1989

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RX(14) OF 14

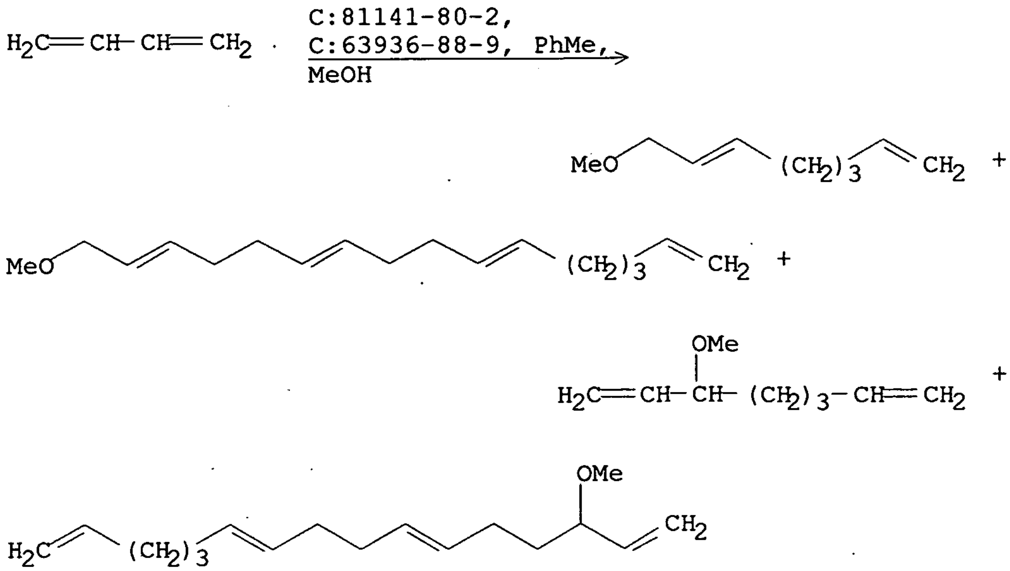
$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow{\text{AcOH, Pd(OAc)2, PhMe}}$

$AcO{-}CH_2{-}CH{=}CH{-}(CH_2)_3{-}CH{=}CH_2$ (68%) + $H_2C{=}CH{-}CH(OAc){-}(CH_2)_3{-}CH{=}CH_2$ (26%)

REF: Journal of Organic Chemistry, 54(11), 2726-30; 1989

L3 ANSWER 43 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

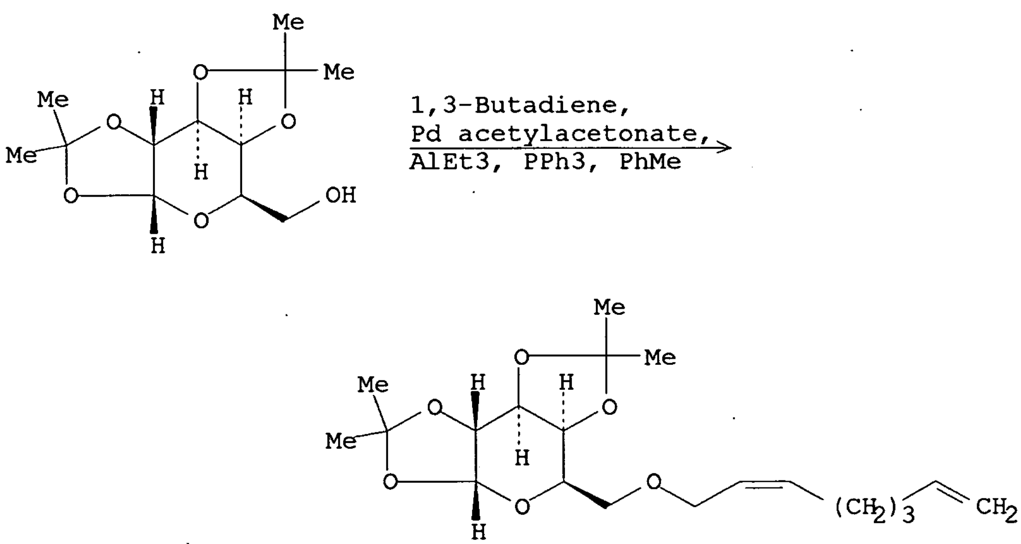
RX(1) OF 19



REF: Journal of Organic Chemistry, 54(10), 2459-62; 1989

L3 ANSWER 44 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3



73%

REF: Zhurnal Organicheskoi Khimii, 24(1), 119-21; 1988

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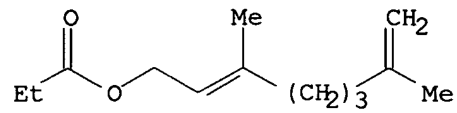
RX(6) OF 6 - 3 STEPS

$H_3C-CH_2-NH-CH_2-CH_3$ $\xrightarrow[\text{2. ClCO2Me; 3. 18-Crown-6, MeCN}]{\text{1. Isopentadiene, PdCl2, PPh3, MeOH}}$



95%

REF: Zhurnal Organicheskoi Khimii, 23(11), 2297-9; 1987

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RX(1) OF 4

$H_2C=CH-CH=CH_2$ $\xrightarrow[\text{NH2OH, PhMe, NMEP}]{\text{Pd acetylacetonate, PPh3, AlEt3, F3CCO2H,}}$

$H_2C=CH-(CH_2)_3-CH=CH-CH_2-OH$ +

$H_2C=CH-(CH_2)_3-CH=CH-CH_2-N(OH)-CH_2-CH=CH-(CH_2)_3-CH=CH_2$ +

$H_2C=CH-(CH_2)_3-CH=CH-CH_2-N(CH_2-CH=CH-(CH_2)_3-CH=CH_2)-CH_2-CH=CH-(CH_2)_3-CH=CH_2$

REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (10), 2254-6; 1986
NOTE: overall yield 51%

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RX(15) OF 20

$H_2N-(CH_2)_3-CO_2H$ $\xrightarrow[\text{Pd acetylacetonate, PhMe, DMSO}]{\text{1,3-Butadiene, AlEt3, PPh3,}}$

$H_2C=CH-(CH_2)_3-CH=CH-CH_2-O-C(=O)-(CH_2)_3-NH_2$

84%

REF: Zhurnal Organicheskoi Khimii, 22(8), 1610-19; 1986

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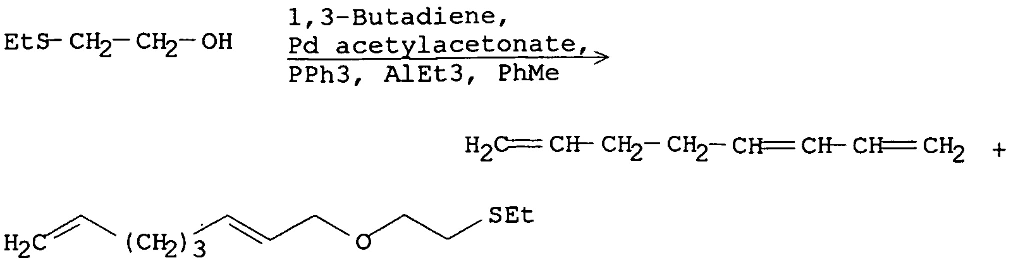
RX(1) OF 20



98%

REF: Zhurnal Organicheskoi Khimii, 22(8), 1591-7; 1986

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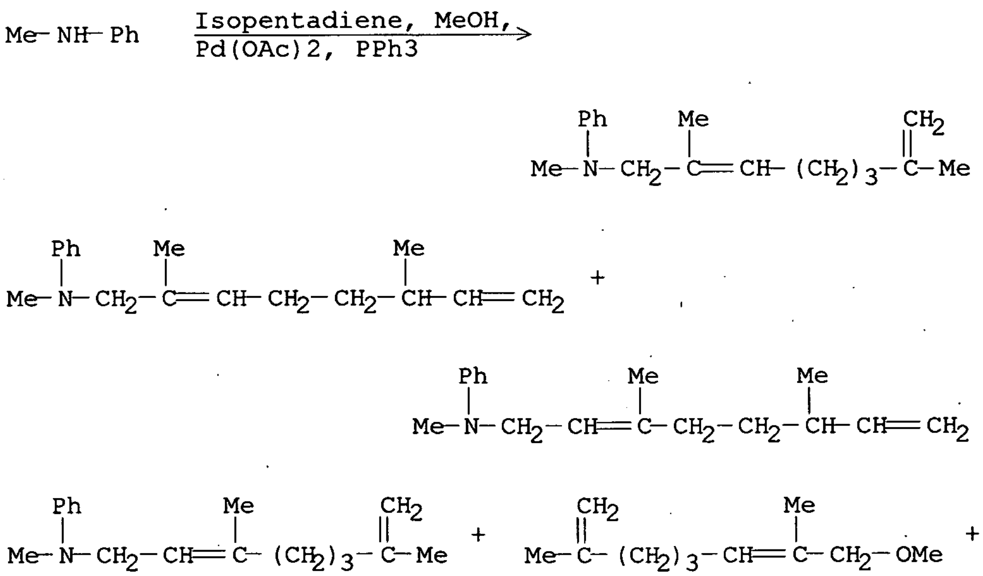
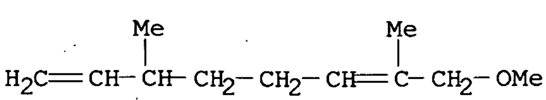
RX(1) OF 14



RX(1) OF 14

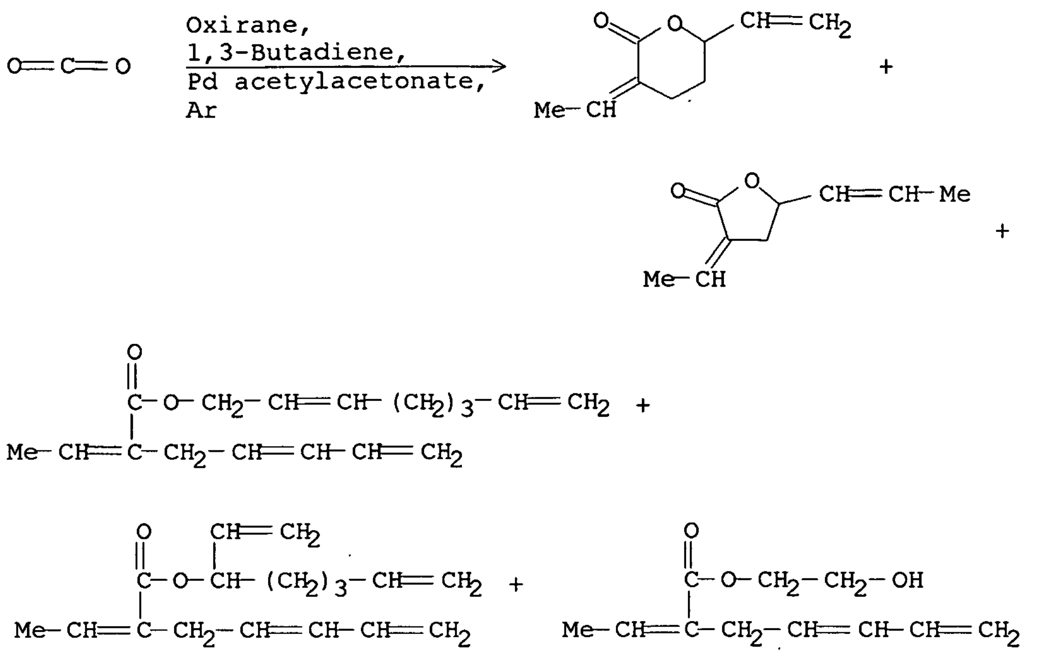


REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (6), 1344-7; 1986

NOTE: or Pd(acac)2

L3 ANSWER 50 OF 68 CASREACT

RX(1) OF 5



REF: Journal of Organometallic Chemistry, 309(1-2), 215-23; 1986

L3 ANSWER 51 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 2

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow{MeOH} H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OMe$

REF: U.S., 4642392, 10 Feb 1987

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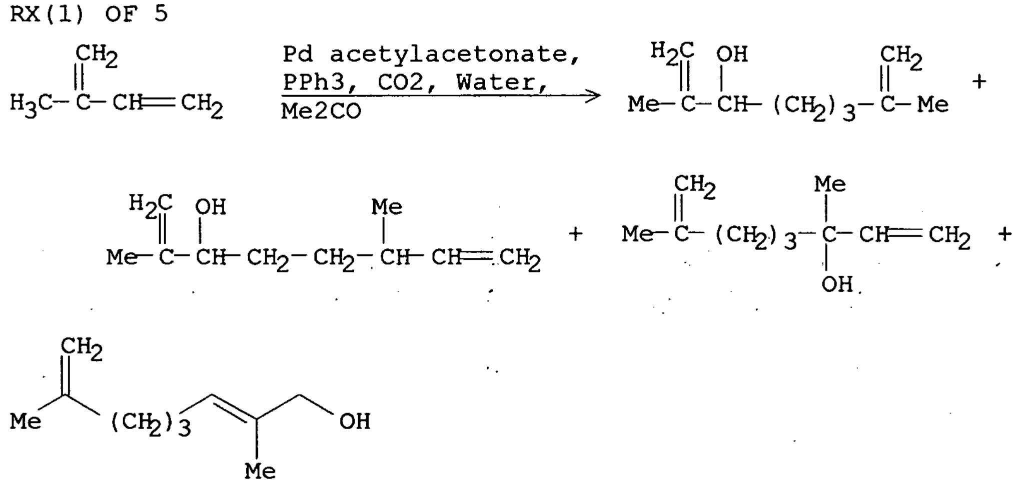
RX(1) OF 5

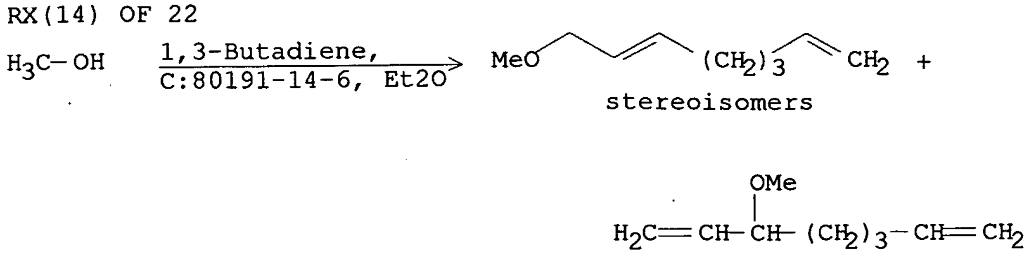


stereoisomers

REF: Zeitschrift fuer Chemie, 25(6), 226-7; 1985

L3 ANSWER 53 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

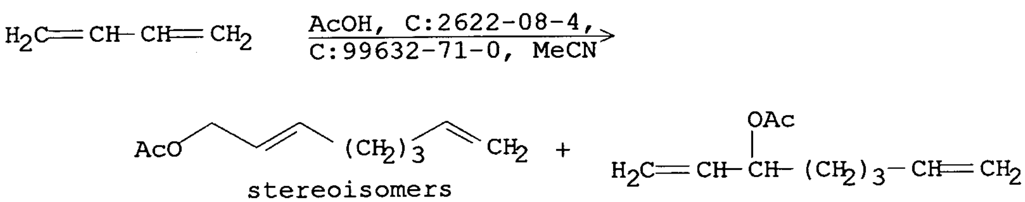
RX(14) OF 22



REF: Organometallics, 5(3), 473-81; 1986

L3 ANSWER 54 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

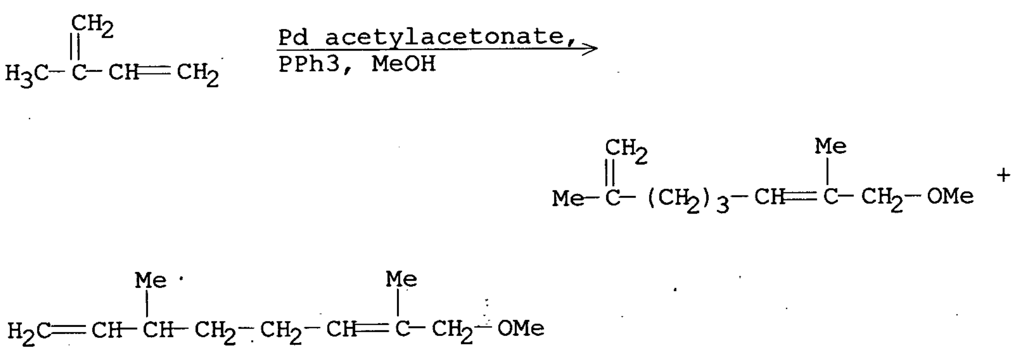
RX(8) OF 21



REF: Organometallics, 5(3), 514-18; 1986

L3 ANSWER 55 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 2



REF: Journal fuer Praktische Chemie (Leipzig), 327(4), 643-8; 1985

L3 ANSWER 56 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

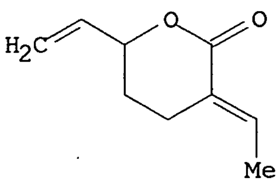
RX(2) OF 16

O=C=O $\xrightarrow[\text{Pd(OAc)2, PPh3, DMF}]{\text{1,3-Butadiene,}}$

$H_2C{=}CH{-}CH_2{-}CH_2{-}CH{=}CH{-}CH{=}CH_2$ +

$AcO{-}CH_2{-}CH{=}CH{-}(CH_2)_3{-}CH{=}CH_2$ +

$H_2C{=}CH{-}CH{=}CH{-}CH_2{-}C({=}CH{-}Me){-}CO_2H$ + $H_2C{=}CH{-}CH(OAc){-}(CH_2)_3{-}CH{=}CH_2$ +



REF: Nippon Kagaku Kaishi, (3), 533-6; 1985

L3 ANSWER 57 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(7) OF 12

$H_2C{=}CH{-}CH{=}CH_2$ $\xrightarrow{\text{MeOH, Pd, Benzene}}$

$H_2C{=}CH{-}(CH_2)_3{-}CH{=}CH{-}CH_2{-}OMe$ +

$H_2C{=}CH{-}CH_2{-}CH_2{-}CH{=}CH{-}CH{=}CH_2$ + $H_2C{=}CH{-}CH(OMe){-}(CH_2)_3{-}CH{=}CH_2$

REF: Journal of Molecular Catalysis, 29(1), 99-104; 1985

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RX(3) OF 3

$H_3C{-}C({=}CH_2){-}CH{=}CH_2$ $\xrightarrow[\text{Me2CHOH}]{\text{MeOH, PBu3, NaOMe,}}$

$Me{-}C({=}CH_2){-}(CH_2)_3{-}CH{=}C(Me){-}CH_2{-}OMe$

REF: Journal fuer Praktische Chemie (Leipzig), 326(5), 729-36; 1984

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RX(1) OF 6

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow{NaOPh} PhO{-}CH_2{-}CH{=}CH{-}(CH_2)_3{-}CH{=}CH_2$

REF: U.S.S.R., 892851, 15 Jul 1982

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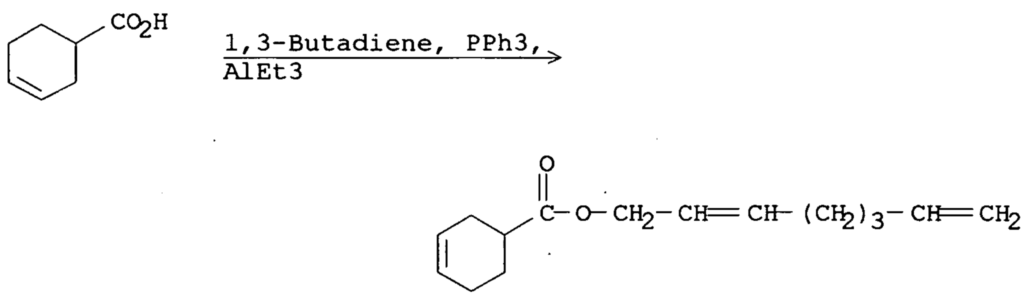
RX(1) OF 15

$H_2C{=}CH{-}CH{=}CH_2 \xrightarrow{PhOH} PhO{-}CH_2{-}CH{=}CH{-}(CH_2)_3{-}CH{=}CH_2$

REF: Angewandte Chemie, 94(10), 796-7; 1982

L3 ANSWER 61 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3

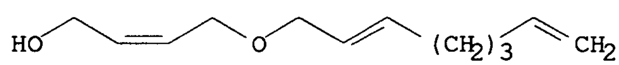


REF: Zhurnal Organicheskoi Khimii, 18(1), 46-52; 1982

L3 ANSWER 62 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(11) OF 12

$HO{-}CH_2{-}CH{=}CH{-}CH_2{-}OH \xrightarrow{\text{1,3-Butadiene}}$

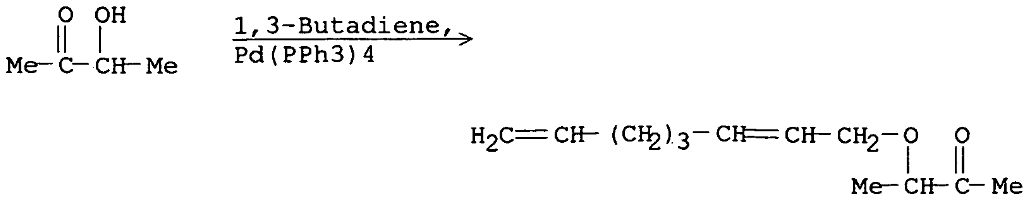


39%

REF: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, (8), 1837-42; 1981

L3 ANSWER 63 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(5) OF 12



REF: Tetrahedron Letters, 21(39), 3787-90; 1980

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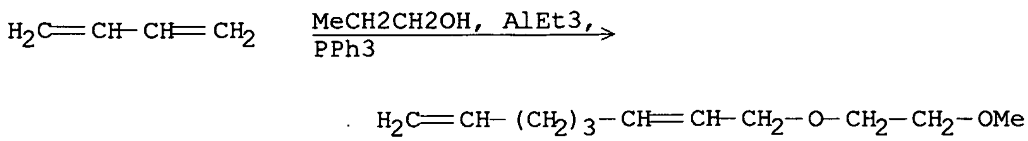
RX(1) OF 6



REF: Zhurnal Organicheskoi Khimii, 16(6), 1157-61; 1980

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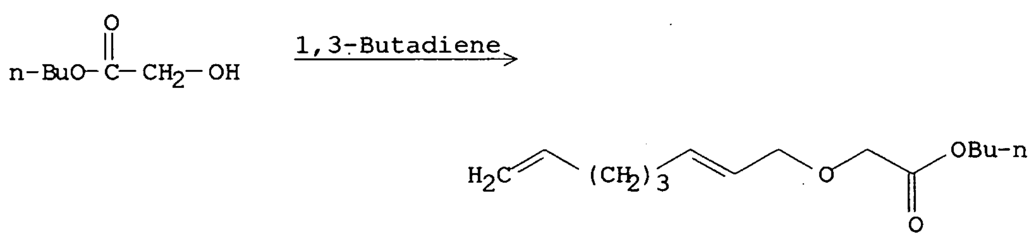
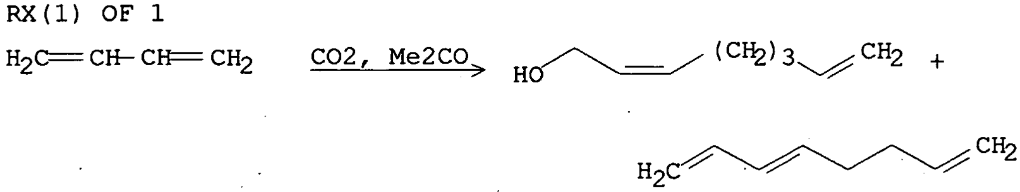
RX(2) OF 10



REF: Journal of Organometallic Chemistry, 137(3), 309-14; 1977

L3 ANSWER 66 OF 68 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 1



REF: Journal of the Chemical Society [Section] D: Chemical Communications, (7), 330; 1971

NOTE: Classification: C-Alkylation; Addition; Hydroxylation; # Conditions: CO2 Pd complex acetone; 90 deg 2h; # Comments: 69% yield of 1-OH product, 13% yield of alkene; 10% yield of octadienyl esters

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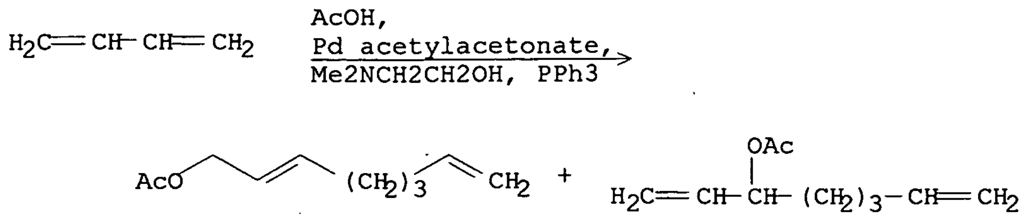
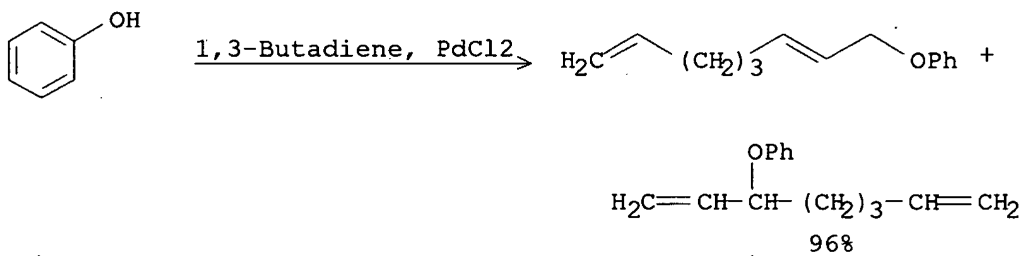
RX(1) OF 1



REF: Tetrahedron Letters, (43), 3817-20; 1970
NOTE: Classification: C-Alkylation; Regioselective; Addition; Acetoxylation; # Conditions: Me2NCH2CH2OH; PPh3 Pd(acac)2; # Comments: 71% yield of 1-OAc product, 21% yield of 3-OAc product; 8% yield of alkene product

L3 ANSWER 68 OF 68 CASREACT

RX(1) OF 4



REF: Journal of the American Chemical Society, 89(25), 6793-4; 1967
NOTE: Classification: Dimerisation; Addition; O-Alkylation; # Conditions: PdCl2 PhONa; 100 deg; # Comments: 91% of trans product